Orthoformic acid, cyclic 2,2-dimethyltrimethylene ethyl ester 5783-79-9 | DTXSID20206542

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.10

Global applicability domain: Inside

Local applicability domain index: 5.68e-01

Confidence level: 5.95e-01

Nearest Neighbors from the Training Set

Image not found

Metaldehyde acetaldehyde

tetramer

Measured: 0.12 Predicted: 4.47e-01

Image not found

Ethyl orthoformate

Measured: 1.20

Predicted: 1.05

Image not found

Paraldehyde Measured: 0.67

Predicted: 8.50e-01

Image not found

Propane, 1,1,1-triethoxy-

Measured: 1.97 Predicted: 1.85

Image not found

Methyl pivalate
Measured: 1.83
Predicted: 1.76